ELSEVIER

Journal of Molecular Liquids 65/66 (1995) 437–439

journal of MOLECULAR LIQUIDS

Author Index

Aicart, E., 195
Amakasu, Y., 377
Asano, Y., 41

Bader, J.S., 31
Barnes, A.C., 99
Barthel, J., 177
Benko, J., 261
Berg, M., 301
Berne, B.J., 31
Blakey, D.M., 85
Bosse, J., 429
Bout, D.V., 301
Buchner, M., 157
Burger, K., 213

Chigira, F., 265
Chikaki, S., 325
Chong, S.-H., 345

Dore, J.C., 85
Dorfmüller, T., 157

Enderby, J.E., 99
Espenson, J.H., 205

Friedman, H.L., 7, 15
Fujimura, Y., 169
Fujiwara, A., 187
Fukuda, T., 341
Fukuda, Y., 397
Fukushima, K., 369
Funahashi, S., 277

Gardecki, J., 49
Goto, M., 357
Gotoh, T., 341
Gyuresik, B., 213

Hamada, S., 353
Hamaguchi, H., 417
Hashimoto, N., 41
Hattori, S., 357
Hayashi, S., 405
Haymet, A.D.J., 139
Hirata, F., 15, 345, 381
Hirata, Y., 321, 421
Hirota, N., 401, 425
Hiwatari, Y., 123
Horng, M.L., 49
Hosoya, K., 305

Ibuki, K., 385
Iida, M., 269
Ikeuchi, H., 273
Irisa, M., 381
Itoh, S., 373
Iwadate, Y., 369
Iwata, K., 417

Jobe, D.J., 195
Johnson, A.E., 59

Kagayama, N., 277
Kai, Y., 413
Kameda, Y., 305
Kanakubo, M., 273
Kanato, H., 325
Kaneko, Y., 429
Kanemoto, Y., 421
Kataoka, Y., 329
Kato, T., 405
Kawaizumi, F., 377
Keogh, G.P., 389
Kimura, Y., 425
Kinoshita, S., 413
Kitagawa, T., 317

Kitahara, K., 293
Kitazawa, M., 321
Koda, S., 337
Koyama, Y., 369
Kubo, H., 369

Ma, J., 301
Machida, K., 405
Madden, P.A., 373
Maeda, H., 341
Maroncelli, M., 49
Mashita, T., 341
Masuda, A., 397
Masuda, Y., 269, 397
Mataga, N., 393
Matsui, J., 123
Matsumoto, M., 277, 329
Matsuoka, T., 337
Matsuura, H., 313
Miyasaka, H., 393
Miyazaki, F., 357
Mizoguchi, K., 187
Mizuno, Y., 269
Morita, A., 75
Moya, M.L., 261
Munakata, T., 15, 131
Murakami, M., 433
Muranaka, T., 123

Nagaoka, M., 289
Nagasawa, Y., 59
Nagy, L., 213
Nakagaki, R., 353
Nakahara, M., 149
Nakai, T., 365
Nakamori, T., 269
Nakamura, K., 341
Nakanishi, K., 281
Nakashima, S., 317
Nakazawa, T., 353
Neilson, G.W., 99
Newton, M.D., 7
Nishinaka, M., 333
Nishiyama, K., 41
Nomoto, T., 421
Nomura, H., 337, 377

Odagaki, T., 123
Ohba, M., 377
Ohtaki, H., 1

Ojima, H., 341
Okada, I., 309
Okada, T., 41, 321, 421
Okako, N., 369
Okamoto, K., 401
Okazaki, S., 309
Olson, J.S., 317
Olsson, L.-F., 349
Ozutsumi, K., 361

Papazyan, A., 49
Perez-Tejeda, P., 261
Perng, B.-C., 7

Radnai, T., 229
Raineri, F., 15
Raineri, F.O., 7
Rick, S.W., 31
Rossky, P.J., 23

Sagawa, T., 313
Sakamoto, S., 305
Sanchez, F., 261
Sasaki, S., 341
Sasaki, Y., 253
Satô, G.P., 273
Sawada, K., 265
Sawai, N., 353
Sawamura, S., 365
Schröer, W., 107
Schwartz, B.J., 23
Seki, K., 293
Seo, Y., 433
Shibata, T., 337
Shinozaki, K., 357
Soper, A.K., 91
Stuart, S.J., 31
Suga, H., 115
Sumi, H., 65
Suzuki, H., 305
Swaddle, T.W., 237

Tabata, M., 221
Takagi, H.D., 277
Takahashi, T., 381
Tanaka, H., 285
Tanida, H., 409
Taniguchi, Y., 365
Tarumi, T., 277
Teramoto, Y., 281

Terauchi, N., 309
Terazima, M., 401
Tominaga, K., 59, 389
Tominaga, T., 333
Tominaga, Y., 187
Tran-Cong, Q., 325
Tsukahara, K., 353

Uemura, O., 305
Ueno, M., 385
Usuki, T., 305

Verrall, R.E., 195

Wakai, C., 149
Wakita, H., 91
Wang, Y., 187
Watanabe, I., 245, 409
Weingärtner, H., 107

Yabe, T., 321
Yagi, T., 413
Yamabe, T., 289
Yamagami, M., 91
Yamaguchi, M., 413
Yamaguchi, T., 91
Yamanaka, M., 341
Yanagida, T., 381
Yartsev, A., 59
Yasuoka, K., 329
Yokoyama, H., 357
Yoshida, N., 289
Yoshihara, K., 59, 389
Yoshimori, A., 297

ELSEVIER Journal of Molecular Liquids, 65/66 (1995) 441–446

journal of MOLECULAR LIQUIDS

Subject Index

absorption curve, 179
acetone solutions, 178
acetonitrile(AN), 13, 18, 177, 180
adiabatic calorimeter, 116
air/solution interface, 250
alkyl radicals, 205
alkylammonium salts, 109
amorphous ice, 85, 87, 89
anharmonic free energy, 286
approximate correlation function, 161
aprotic dipolar liquid, 18, 19
aqueous CsCl solution, 365
aqueous electrolyte solutions, 187
aqueous solution of NaCl at high pressure, 233
aqueous solutions, 91, 229
aqueous solvation, 31
aqueous sulfuric acid solutions, 305
argon, 329
argon/a-ice co-deposit, 88
Argand diagram, 181, 182
ascorbic acid, 187, 277
association constant, 177, 179, 184
average distances, 232
avian pancreatic polypeptide, 381
azobenzene, 65

benzene, 13, 273
N-benzylideneanilines, 65
biferrocene monocation, 397
bimolecular reaction rate, 321
binary soft-sphere mixtures, 121
bipyridine, 357
bi-exponential decay, 19, 20
Born-Mayer-Huggins, 373
bromide ion, 230, 245
Brownian motion, 75
butanol, 199
1-butoxyethanol, 199

calcium, 349
Car-Parrinello method, 373
carbonmonoxy myoglobin, 317
catalytic effect, 222
$CeCl_3$, 369
central component, 187
central force (CF) model, 139
CD, 213
CF_3H, 313
charged ion pairs, 184
chloride ion, 230
classical (continuum) model of solvent, 261
clathrate, 89, 118, 185
closest approach, 265
cluster form-factor, 87
$[Co(NH_3)_4(pzCO_2)]^{2+}$, 261
cobalt (III) ammine complexes, 237
coherent anti-Stokes Raman profiles, 169
Cole-Cole plots, 125
Cole-Cole type relaxation mode, 187
collective jump motions of atoms, 123
collective variables, 15
collectivity, 157
^{59}Co longitudinal relaxation rates, 273
combination reaction, 207
complexes of N-D-gluconylamino acids, 213
computer simulation, 329
condensation coefficent, 329
conductivity, 265, 357
configurational enthalpy, 120
conformational behavior, 313
conformational fluctuations, 65
contact ion pair(s), 177, 184
continuous random network, 87
continuum model, 385
coordination distance, 245
coordination numbers, 232, 245
correlated atomic diffusion model, 15
correlated motion coefficient, 127
correlation time, 433
corresponding state, 109
Coulombic phase separations, 108
cresyl violet, 41
critical behavior, 107
critical density, 425
crossover, 107
crystalline solids, 115
crystallization, 115
Cu(II) porphyrin complex, 231
9-cyanoanthracene-1, 3-cyclohexadine, 321

Debye type relaxation mode, 187

density autocorrelation function, 123
density correlation, 16
density fluctuations, 131
density functional (method), 16, 281
density functional theory, 131
density maximum, 86
density of state, 162
dependence of relaxation rate on the temperature, and the complex concentration, 273
dephasing, 131
dephasing constant, 169
detailed balance, 293
di- and tri-nuclear complexes, 253
diabatic free energy profiles, 8
dichrolomethane, 273
dielectric constant, 114
dielectric depression, 182
difference pair-distribution function, 233
diffusion coefficients, 333
diffusion constant, 17
diffusion controlled reactions, 184
diffusion mechanism, 429
diffusion-controlled rate constant, 207
diffusive Browinan motions, 65
diffusive motions, 65
N, N-dimethylformamide, 180, 229, 361
dimethyle suifoxide solutions, 227, 230, 178
dipolar and non-dipolar (polar) solvents, 7
dipole-dipole interaction, 409
direct correlation, 16
discrete-exchange model, 435
dispersion amplitude, 181
dispersion curve, 179
disproportionation, 205
dissipative structure, 341
dissociation pressure, 286
DLVO approximation, 139
double-quantum filter NMR, 434
dropping effect, 118
dye, 59
dynamic effect, 289
dynamic process in electrolyte solutions, 177
dynamic variables, 15
dynamical nonlinear terms, 297
dynamical structure factor, 15, 16
dynamical structure of water, 187
dynamics, 91
dynamics of solvation, 49
$d\pi - p\pi$ interactions, 253

effective dipole moments, 184
effective ionic radius, 358
effective volume of dipole rotation, 184
electric field gradients, 269
electrolyte solutions, 107
electron donors, 209
electron exchange rate, 209
electron transfer, 59
electron transfer reaction(s), 7, 205, 237, 345
electrostriction, 359
encounter pair, 321
energetics, 211
energy transfer, 405
enthalpy change of the ion association, 358
enthalpy relaxation, 120
entropy change of the ion association, 358
EPR, 213
erbium (III) ions, 230
evaporation and condensation, 329
EXAFS, 230, 245, 213
EXAFS oscillation amplitudes, 247
excess free energy, 357
excimer, 394
excitation energy migration, 393
excition diffusion, 393

$[Fe(CN)_6]^{4-}$, 261
femtosecond, 59
femtosecond time-resolved coherent Raman scattering, 169
finger-like structure flow, 341
first excited singlet, 417
first- order difference method, 230
fluctuation dissipation theorem, 18, 414
fluorescence quenching, 321
fractional exponent, 116
free energy profiles, 7, 11
free-volume, 325
friction kernel, 16
frozen-in systems, 115
FT-IR spectroscopy, 177, 313
functional derivative, 16

general susceptibilty, 123
generalized Langevin equation, 15, 289

generalized permittivity, 179
glass transition, 115, 126, 429
glassy, 91
glassy crystals, 115
glassy polymers, 325
glassy water and solutions, 231
D-glucose solution, 187
Gouy-Chapman-Stern (GCS) approximation, 139
Grote-Hynes theory, 65, 289
ground state recovery, 425

halogen abstraction, 205
hard-sphere liquid, 429
heat capacity, 118
heat capacity change of the ion association, 358
heat conduction, 417
heat transfer, 331
heavy water, 149
heterodinuclear metalloporphyrin, 221
hexagonal $ErCl_3$, 369
high frequency permittivity, 177, 179
high pressure, 365
homogeneous solvent, 18
homogeneous and inhomogeneous contributions, 389
homogenisation, 158
^1H relaxation, 269
^1H spin-lattice relaxation, 397
hydrated electron, 23
hydration, 91, 357
hydration entropy and enthalpy, 360
hydration free energy, 381
hydrogen abstraction reaction, 401
hydrogen atom abstraction, 205
hydrogen bond, 18, 91, 149
hydrogen carbonate, 349
hydrogen-bond connectivity, 89
hydrogen-bond formalisim, 409
hydrogen-bonded intermolecular structure, 305
hydrogen-bonded pair, 86
hydrophobic, 177, 357
hydrophobic complex, 359
hydrophobic interaction(s), 182, 357
hydrophobic structure-makers, 357
hyper-quenced glassy water, 87

inorganic reaction mechanism, 237
instantaneous normal modes, 157
integral equation method, 15
integral equation theory, 345, 377
integral motion, 20
interaction site model, 7
intermolecular, 169
intermolecular dephasing, 169
intermolecular interactions, 7, 169
intramolecular electron transfer, 397
intramolecular photodimerization, 325
ion association, 177, 357
ion solvation, 177
ion-aggregate formation, 177
ion-association theory, 360
ion-pair formation, 265, 358
ion-pair relaxation, 184
ion-pairing effects, 269
ionic atmosphere, 333
ionic products, 212
irrotational bonding, 182
isochoric temperature derivative, 86, 87
isolobal, 205
isomorphic replacement, 230
isotropic substitution, 99

Jones-Dole B coefficient, 365, 385

kinetic depolarization, 182
kinetic relaxation process, 184
Kohlrausch-Williams-Watts' equation, 116
Kramers theory, 65

Langevin-diffusion equation, 131
laser flash photolysis, 205
Lennard-Jones binary mixture, 377
LiCl solution in DMF, 232
light scattering, 113, 413
limiting molar conductivity, 265
linear response, 19, 261
LiNCS solution in DMF, 232
liquid, 91, 169
liquid acetonitrile, 235
liquid benzene, 393
liquid crystal, 281
liquid surface, 330
liquid-liquid phase separation, 107
lithium halides, 91
lithium iodide (LiI), 373
lithium ion, 229

local relaxation processes, 325
localization transition, 429
long time limit of the reaction, 75
low-frequency Raman scattering, 187

Marcus equation, 209
Marcus-Hush theory, 237
Markov limit, 16
MD simulation, 17, 229, 286, 329, 405
mean-field-like criticality, 107
mechanical grinding, 120
mechanical relaxation theory, 301
melting behavior, 369
metal radical, 205
metal-to metal charge transfer, 261
metalloporphyrin, 221
metastable phase, 115
methanol, 18, 329
methyl chlorides, 18
$MgCl_2$-water-methanol ternary systems, 231
micelle, 333
microscopic Hamiltonian, 289
microscopic viscosity, 385
mixed micelles, 196
mixed-valence, 253, 397
mode coupling theory, 301
mode-coupling theory, 429
molecular liquids, 131
molecular theory of solvation dynamics, 7
molybdenum radical, 209
momentum density, 15
monoclinic ErCl3, 369
monohalogenocadmium (II) complexes, 361
Monte Carlo (MC) computer simulation, 229
Mossbauer structual study, 213
multi-exponential behavior, 17
multi-exponential decay, 17
MW spectra, 177

^{23}Na NMR, 433
N_2O_4, 405
naphthalenedisulfonates, 360
neutron diffraction, 85, 99
neutron scattering, 91
neutron scattering, 99
new renormalized linear response development, 7
nickel (II) and magnesium (II) ions, 230
nitrate ions, 230
NMR, 149, 213
NMR relaxations, 20, 269
non-adiabatic relaxation, 23
non-aqueous solutions, 229
non-crystalline solids, 115
non-exponential relaxation, 116
nonlinear coupling terms, 289
nonlinear Smoluchowski-Vlascov equation, 297
normal mode spectra, 158

octadecyltrimethylammonium chloride, 333
open form, 317
optical Kerr effect, 413
organic free radicals, 208
organic halides, 208
organometallic free radical, 205
orientational structure, 158
Ornstein-Zernike equation, 378
oxidation, 277
oxide bridge, 253

pair correlation function(s), 85, 86, 88
partial molar volumes, 358
partial pair-distribution function, 235
partial specific volumes, 341
pentanone, 199
perchlorate (ion), 230, 357
phenanthroline, 357
phenol blue, 425
photoelectron emission spectroscopy, 409
photoexecitation, 15, 18, 23
photohomolysis, 205
photophysical properties, 353
physiological solutions, 349
picosecond laser photolysis, 393
picosecond time-resolved Raman spectroscopy, 417
POE-water system, 313
Poisson-Boltzmann equation, 381
polar and non-dipolar solvents, 7
polar liquid, 15, 18
polarizability, 373
polarizable, 31
polarization charge density, 15
poly (oxyethylene) (POE), 313
polypeptide, 381
porphylin, 221

potential height, 81
power spectra, 286
precipitation nuclei, 349
pressure effects on reaction, 237
propanol, 199
propylene carbonate (PC), 180, 301
protein, 381
protein dynamics, 317
proton transfer, 209
pulsed field gradient NMR, 434
PY approximation, 377

quadrupole coupling constant, 433
quantum molecular dynamics, 23
quasi-elastic neutron scattering (QENS), 99, 230

radical, 401
Raman echo experiment, 389
Raman spectra, 305
Raman spectroscopy, 187, 309
rapid transport of a polymer, 341
rate constants, 196
rate of chemical reactions, 81
recombination, 211
recombination process, 317
redox properties, 253
relaxation, 115
relaxation mode, 187
relaxation of inhomogeneity, 425
relaxation process, 180
relaxation time, 116, 180
relaxation time distribution, 180
relaxation times in fluid solution, 41
renormalized solute-solvent interactions, 8
reorganization energy, 7, 409
reorientation dynamics, 325
residuasl entropy, 115
response function, 180
reverse Monte Carlo simulation, 229, 234
rhodium radical, 208
RISM, 10, 15, 16
root mean square deviations, 232
rotational and vibrational relaxation, 309
rotational correlation times, 149
rotational diffusion, 421
rotational friction coefficient, 385
rundom force, 16

S_1-S_1 annihilation, 394

scaled particle theory, 381
scattering, 169
Schlogl model, 293
second order difference method, 230
self-diffusion coefficient, 433
self-exchange reaction rate, 239
short range structure, 369
short-lived intermediates, 221
silver ion, 230
single-particle dynamics, 159
singlet excitation energy transfer, 393
site dependent relaxation time, 48
site-number density, 15, 18
site-site Smoluchowsky-Vlascov (SSSV) equation, 15, 19, 21
small angle neutron scattering (SANS), 230
small model of gilcoproteins, 213
Smoluchowski equation, 75
sodium (I) ion, 230
sodium chloride, 229
solid-fluid interface, 281
solid-state amorphization, 120
solution reactions, 65
solvate structure, 229
solvation, 23, 177
solvation dynamics, 10, 15, 297, 301
solvation free energy, 7, 381
solvation numbers, 177
solvation numbers, 178
solvation of lithium ion in N, N-dimethyl formamide, 231
solvation structure, 245
solvation time, 59
solvation time correlation function (STCF), 18, 19, 20
solvent dynamical effect, 397
solvent exchange, 238
solvent orientational distribution, 48
solvent pressure effect, 149
solvent relaxation, 41
solvent separated ion pair, 177
solvent viscosity, 65
solvent-solute interaction, 421
solvophobic unmixings, 111
spatial correlations, 293
SPC model, 17, 19
stability of ion pairs, 177
stearyltrimethylammonium bromide, 250
sticky ions, 111
trans-stilbene, 417

Stokes radius, 265, 358
Stokes-Einstein-Debye law, 149
stopped flow EXAFS experiment, 231
stretched exponential function, 123
structual parameters, 232
structure, 91, 361
structure and dynamics of solvated ions, 229
structure of coordination of isomers, 219
structure-breaker, 359
structure-makers, 367
Sumi and Marcus, 65
supercooled, 91, 231
supercooled liquids, 131
supercooled fluid phase, 123
supercritical fluid, 309
supersaturated aqueous solutions, 349
surfactant-alcohol, 196

temperature coefficients of the Walden product, 358
temperature pressure effect, 149
temperature dependence of molar conductivities, 357
tetraalkylammonium, 265
n-tetradecyltrimethylammonium bromide, 333, 337
tetramethyl urea, 231
s-tetrazine, 301
theory of solvation dynamics, 7
thermal dissociation, 405
thermochemistry, 211
thermodynamic derivatives, 377
time correlation function of solvent fluctuation, 46
time evolution of the ground state hole, 41
time resolved absorption spectroscopy, 41
time resolved fluorescence spectroscopy, 41
time resolved hole burning, 41
time resolved resonance Raman, 317
time resolved Stokes shift, 18
time-of-flight (TOF) neutron diffraction, 305
TIPS model, 19
tracer diffusion, 333
transient, 205
transient effect in the fluorescene decay curves, 321
transient grating, 401
transient hole burning, 301
transition metal complexes, 237
transition-state theory, 289
translational diffusion, 401
translational friction coefficient, 385
transport coefficents, 131
transport of linear polyelectrolytes, 341
transport properties, 385
transverse relaxation rate constants, 433
trajectory, 17
triatomic molecule, 281
trifluoroethanol, 231
trifluoromethane, 425
tris(1, 10-phenanthroline)ion(II), 357
tri-exponential decay, 19
tungsten, 208

ultrasonic absorption, 195
ultrasonic relaxation method, 337
under-cooled liquids, 87

van der Waals and Platteeuw theory, 285
vapor deposition, 119
variances, 197
velocity correlation function, 157
vertical energy gap, 7, 9
vibrational colling, 417
vibrational lineshape, 389
viologen-linked N-alkylporphyrins, 353
viscosity, 187, 365
viscosity correlation functions, 286
volume change, 369
volume of activation, 238

XANES, 230
X-ray, 305
X-ray diffraction, 91, 229, 361
α - peak, 123
α - relaxation, 123
β - relaxation, 123